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LOGINID:sssptau121zxn

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

| | | |
|---|---|---|
| NEWS 1 | | Web Page URLs for STN Seminar Schedule - N. America |
| NEWS 2 | | "Ask CAS" for self-help around the clock |
| NEWS 3 | May 12 | EXTEND option available in structure searching |
| NEWS 4 | May 12 | Polymer links for the POLYLINK command completed in REGISTRY |
| NEWS 5 | May 27 | New UPM (Update Code Maximum) field for more efficient patent SDIs in CAplus |
| NEWS 6 | May 27 | CAplus super roles and document types searchable in REGISTRY |
| NEWS 7 | Jun 28 | Additional enzyme-catalyzed reactions added to CASREACT |
| NEWS 8 | Jun 28 | ANTE, AQUALINE, BIOENG, CIVILENG, ENVIROENG, MECHENG, and WATER from CSA now available on STN(R) |
| NEWS 9 | Jul 12 | BEILSTEIN enhanced with new display and select options, resulting in a closer connection to BABS |
| NEWS 10 | Jul 30 | BEILSTEIN on STN workshop to be held August 24 in conjunction with the 228th ACS National Meeting |
| NEWS 11 | AUG 02 | IFIPAT/IFIUDB/IFICDB reloaded with new search and display fields |
| NEWS 12 | AUG 02 | CAplus and CA patent records enhanced with European and Japan Patent Office Classifications |
| NEWS 13 | AUG 02 | STN User Update to be held August 22 in conjunction with the 228th ACS National Meeting |
| NEWS 14 | AUG 02 | The Analysis Edition of STN Express with Discover! (Version 7.01 for Windows) now available |
| NEWS 15 | AUG 04 | Pricing for the Save Answers for SciFinder Wizard within STN Express with Discover! will change September 1, 2004 |
| NEWS 16 | AUG 27 | BIOCOMMERCE: Changes and enhancements to content coverage |
| NEWS 17 | AUG 27 | BIOTECHABS/BIOTECHDS: Two new display fields added for legal status data from INPADOC |
| NEWS 18 | SEP 01 | INPADOC: New family current-awareness alert (SDI) available |
| NEWS 19 | SEP 01 | New pricing for the Save Answers for SciFinder Wizard within STN Express with Discover! |
| NEWS 20 | SEP 01 | New display format, HITSTR, available in WPIDS/WPINDEX/WPIX |
| NEWS 21 | SEP 14 | STN Patent Forum to be held October 13, 2004, in Iselin, NJ |

| | |
|---|---|
| NEWS EXPRESS | JULY 30 CURRENT WINDOWS VERSION IS V7.01, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 11 AUGUST 2004 |
| NEWS HOURS | STN Operating Hours Plus Help Desk Availability |
| NEWS INTER | General Internet Information |
| NEWS LOGIN | Welcome Banner and News Items |
| NEWS PHONE | Direct Dial and Telecommunication Network Access to STN |
| NEWS WWW | CAS World Wide Web Site (general information) |

Enter NEWS followed by the item number or name to see news on that specific topic.

* * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 10:53:23 ON 21 SEP 2004

=> FILE REG

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| FULL ESTIMATED COST | 0.21 | 0.21 |

FILE 'REGISTRY' ENTERED AT 10:53:35 ON 21 SEP 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.


Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 20 SEP 2004 HIGHEST RN 748739-98-2
DICTIONARY FILE UPDATES: 20 SEP 2004 HIGHEST RN 748739-98-2

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

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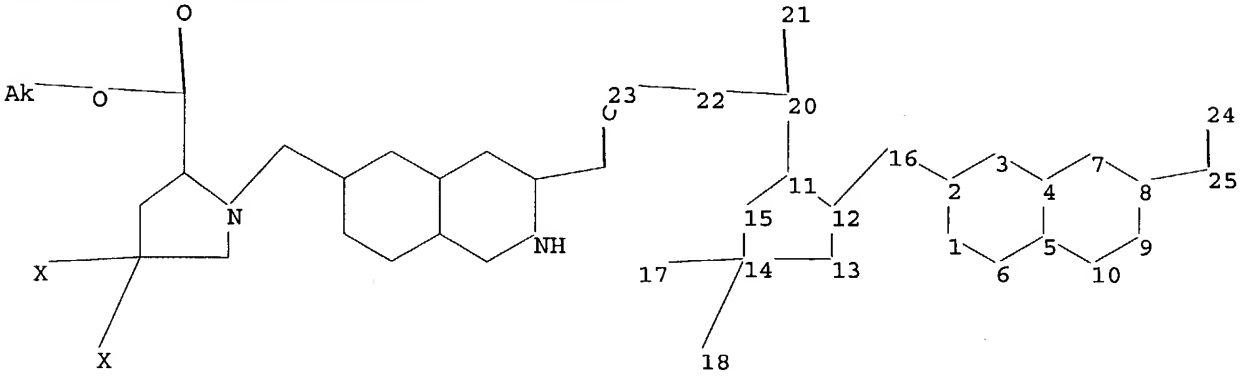


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ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15

```
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ring bonds :
1-2  1-6  2-3  3-4  4-5  4-7  5-6  5-10  7-8  8-9  9-10  11-12  11-15  12-13  13-14
 14-15
exact/norm bonds :
1-2  1-6  2-3  3-4  4-5  4-7  5-6  5-10  7-8  8-9  9-10  11-12  12-13  12-16  20-21
 20-22  22-23  24-25
exact bonds :
2-16  8-25  11-15  11-20  13-14  14-15  14-17  14-18
isolated ring systems :
containing 1 : 11 :


Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:Atom
11:Atom  12:Atom  13:Atom  14:Atom  15:Atom  16:CLASS  17:CLASS  18:CLASS  20:CLASS
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L1                STR
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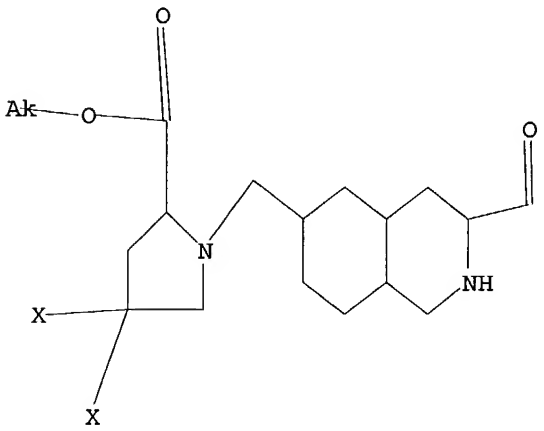


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Structure attributes must be viewed using STN Express query preparation.


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SAMPLE SCREEN SEARCH COMPLETED -      1 TO ITERATE

100.0% PROCESSED       1 ITERATIONS                              1 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:             1 TO       80
PROJECTED ANSWERS:                1 TO       80
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SEARCH TIME: 00.00.01

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COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   155.42     155.63

FILE 'CAPLUS' ENTERED AT 10:54:19 ON 21 SEP 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)
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FILE COVERS 1907 - 21 Sep 2004  VOL 141 ISS 13
FILE LAST UPDATED: 20 Sep 2004  (20040920/ED)

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.


=> s l3
L4            3 L3

=> s l4 and pd<july 1999
      19649264 PD<JULY 1999
                 (PD<19990700)
L5            0 L4 AND PD<JULY 1999

=> dis l4 1-3 bib abs hitstr

L4   ANSWER 1 OF 3  CAPLUS  COPYRIGHT 2004 ACS on STN
AN   2002:521737  CAPLUS
DN   137:78867
TI   Preparation of carboxydifluoropyrrolidinylmethyldecahydroisoquinolinecarbo
     xylates as excitatory amino acid receptor antagonists.
IN   Khau, Vien Van; Letourneau, Michael Edward; Martinelli, Michael John
PA   Eli Lilly and Company, USA
SO   PCT Int. Appl., 54 pp.
     CODEN: PIXXD2
DT   Patent
LA   English
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FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
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| PI | WO 2002053561 | A1 | 20020711 | WO 2001-US44715 | 20011220 |
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| | BR 2001016672 | A | 20030923 | BR 2001-16672 | 20011220 |
| | EP 1351955 | A1 | 20031015 | EP 2001-995980 | 20011220 |
| | R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR | | | | |
| | JP 2004520335 | T2 | 20040708 | JP 2002-554680 | 20011220 |
| | US 2004082606 | A1 | 20040429 | US 2003-450458 | 20030613 |
| | NO 2003002973 | A | 20030627 | NO 2003-2973 | 20030627 |
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OS MARPAT 137:78867

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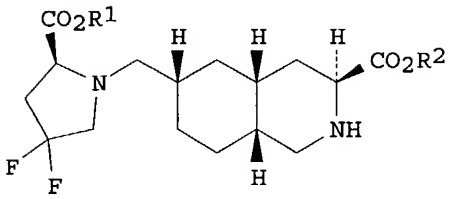


I

AB Pharmaceutically acceptable salts of title compds. (I; R1, R2 = H, alkyl, alkenyl, alkylaryl, alkylcycloalkyl, alkyldiaminoalkyl, alkylpyrrolidinyl, alkylpiperidinyl, alkylmorpholinyl), were prepared A mixture of Et (3S,4aR,6S,8aR)-6-(hydroxymethyl)-2-(methoxycarbonyl)-1,2,3,4,4a,5,6,7,8,8a-decahydroisoquinoline-3-carboxylate and Et3N in EtOAc is added dropwise to p-nitrobenzenesulfonyl chloride in EtOAc at 0-2° followed by warming to room temperature and stirring for 2.5 h to give 97% sulfonate ester. This was refluxed with hydroxyproline Et ester in EtOAc to give an oil, which in CH2Cl2 was added to a -10° mixture of POCl3 and Me2SO in CH2Cl2 to give 41% ketopyrrolidinylmethyldecahydroisoquinoline derivative This was stirred 21 h with deoxofluor [[bis-(2-methoxyethyl)amino]sulfur trifluoride] and EtOH in 1,2-dichloroethane to give 61% difluoropyrrolidinylmethyldecahydroisoquinoline derivative, which was N-deprotected with Me3SiI in CH2Cl2 followed by salification with D-mandelic acid to give Et (3S,4aR,6S,8aR)-6-[[(2S)-2-(ethoxycarbonyl)-4,4-difluoropyrrolidinyl]methyl]-1,2,3,4,4a,5,6,7,8,8a-decahydroisoquinoline-3-carboxylate D-(-)-mandelic acid salt. The dihydrochloride salt of the latter inhibited elec. stimulated dural protein extravasation with ID100 = 0.01 ng/kg orally in rats.

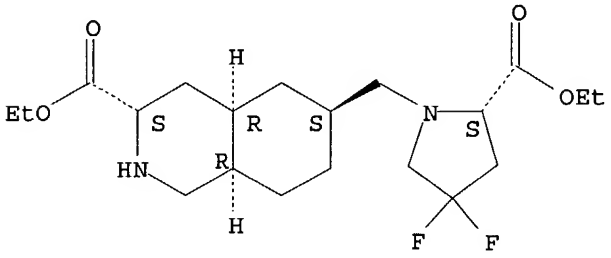
IT **317844-37-4P 440632-08-6P 440632-09-7P**

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU

(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of carboxydifluoropyrrolidinylmethyldecahydroisoquinolinecarboxylates as excitatory amino acid receptor antagonists)

RN 317844-37-4 CAPLUS
CN 3-Isoquinolinecarboxylic acid, 6-[[(2S)-2-(ethoxycarbonyl)-4,4-difluoro-1-pyrrolidinyl]methyl]decahydro-, ethyl ester, dihydrochloride, (3S,4aR,6S,8aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



●2 HCl

RN 440632-08-6 CAPLUS
CN 3-Isoquinolinecarboxylic acid, 6-[[(2S)-2-(ethoxycarbonyl)-4,4-difluoro-1-pyrrolidinyl]methyl]decahydro-, ethyl ester, (3S,4aR,6S,8aR)-, mono[(αR)-α-hydroxybenzeneacetate] (9CI) (CA INDEX NAME)

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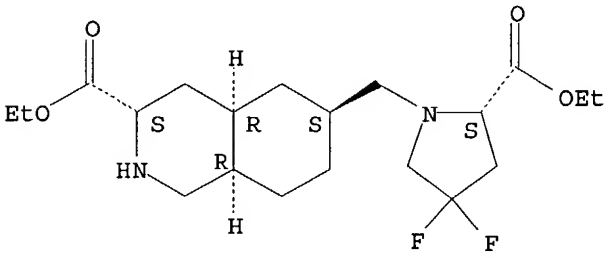
CRN 317844-31-8
CMF C20 H32 F2 N2 O4

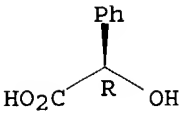
Absolute stereochemistry.



CM 2

CRN 611-71-2
CMF C8 H8 O3

Absolute stereochemistry. Rotation (-).



RN 440632-09-7 CAPLUS
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CRN 317844-31-8
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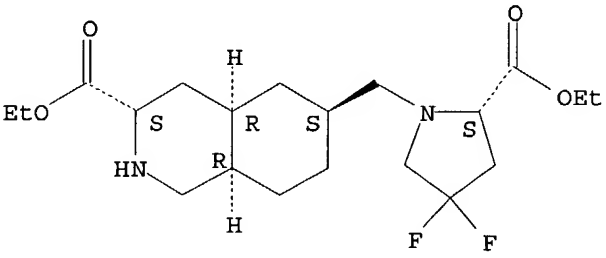
Absolute stereochemistry.



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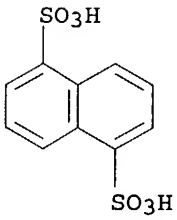

RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:521727 CAPLUS
DN 137:78866
TI Preparation of pyrrolidinyl- and piperidinylmethyldecahydroisoquinolinecarboxylates as excitatory amino acid receptor antagonists.
IN Filla, Sandra Ann; Hudziak, Kevin John; Mathes, Brian Michael; Ornstein, Paul Leslie
PA Eli Lilly and Company, USA
SO PCT Int. Appl., 116 pp.
CODEN: PIXXD2

DT Patent
LA English
FAN.CNT 1

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| PI WO 2002053555 | A2 | 20020711 | WO 2001-US44714 | 20011220 |
| WO 2002053555 | A3 | 20030206 | | |

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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

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R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR

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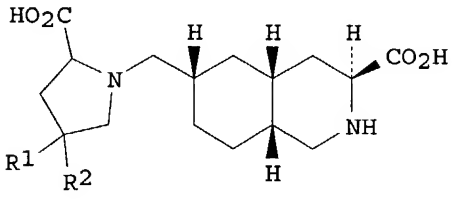
| WO 2001-US44714 | W | 20011220 | |

OS MARPAT 137:78866
GI



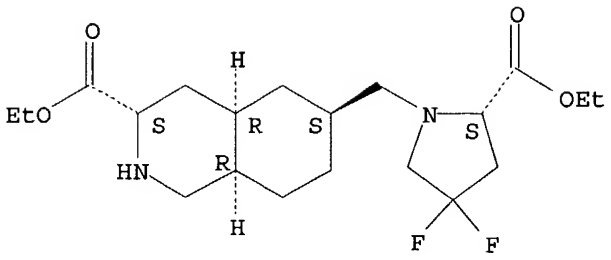

I

AB Title compds. e.g., [I; R1 = H, Cl, Br, iodo, F, SR3, OH; R2 = H, F; R3 = (substituted) tetrazolyl, triazolyl, alkyl, carboxyalkyl; with provisos], were prepared for treatment of e.g., migraine and pain (no data). Thus, Et (3S,4aR,6S,8aR)-6-hydroxymethyl-2-methoxycarbonyldecahydroisoquinoline-3-carboxylate was tosylated followed by coupling with trans-4-OH-L-proline Et ester hydrochloride. The product was oxidized with Me2SO/(COCl)2 in CH2Cl2 followed by fluorination of the resulting ketone with DAST and deprotection with Me3SiCl to give Et (3S,4aR,6S,8aR)-6-[[(2S)-2-(ethoxycarbonyl)-4,4-difluoropyrrolidinyl]methyl]-1,2,3,4,4a,5,6,7,8,8a-decahydroisoquinoline-3-carboxylate.

IT **317844-31-8P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrrolidinyl- and piperidinylmethyldecahydroisoquinolinecarboxylates as excitatory amino acid receptor antagonists)

RN 317844-31-8 CAPLUS
CN 3-Isoquinolinecarboxylic acid, 6-[[(2S)-2-(ethoxycarbonyl)-4,4-difluoro-1-pyrrolidinyl]methyl]decahydro-, ethyl ester, (3S,4aR,6S,8aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2001:31316 CAPLUS
DN 134:91148
TI Selective iGluR5 receptor antagonists for the treatment of migraine
IN Bleakman, David; Chappell, Amy Suzon; Filla, Sandra Ann; Johnson, Kirk Willis; Ornstein, Paul Leslie
PA Eli Lilly and Company, USA
SO PCT Int. Appl., 34 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
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| PI | WO 2001001972 | A2 | 20010111 | WO 2000-US16297 | 20000627 |
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| | HR 2002000013 | A1 | 20030831 | HR 2002-13 | 20020107 |
| | US 2003199546 | A1 | 20031023 | US 2003-383296 | 20030306 |
| | US 6759418 | B2 | 20040706 | | |
| PRAI | US 1999-142485P | P | 19990706 | | |
| | US 1999-151165P | P | 19990827 | | |
| | WO 2000-US16297 | W | 20000627 | | |
| | US 2001-9655 | A1 | 20011211 | | |

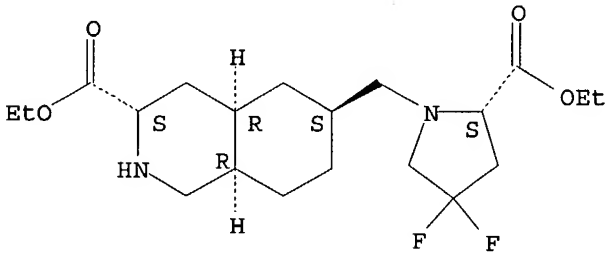
OS MARPAT 134:91148
AB The present invention provides a method of treating or preventing migraine which comprises administering to a patient in need thereof an effective amount of a selective iGluR5 receptor antagonist. The present invention further provides novel compds. functional as selective iGluR5 receptor antagonists, i.e., isoquinoline carboxylate derivs., as well as compns.

and formulations comprising said selective iGluR5 receptor antagonists. Formulations of hard gelatin capsules, tablets, an aerosol solution, suppositories, suspensions, and i.v. injections are provided. For example, i.v. administration of 3S,4aR,6S,8aR-6-(((4-carboxy)phenyl)methyl)-1,2,3,4,4a,5,6,7,8,8a-decahydroisoquinoline-3-carboxylic acid (preparation given) inhibited dural protein extravasation, a functional characteristic of migraine, with ID50 of 6.5 and 4.0 ng/kg in rats and guinea pigs, resp.

IT **317844-31-8P 317844-35-2P 317844-37-4P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of selective iGluR receptor antagonists for treatment of migraine)

RN 317844-31-8 CAPLUS
CN 3-Isoquinolinecarboxylic acid, 6-[[(2S)-2-(ethoxycarbonyl)-4,4-difluoro-1-pyrrolidinyl]methyl]decahydro-, ethyl ester, (3S,4aR,6S,8aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

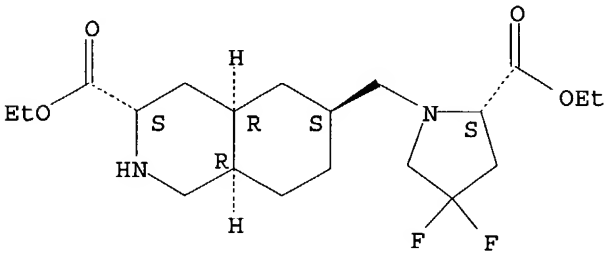



RN 317844-35-2 CAPLUS
CN 3-Isoquinolinecarboxylic acid, 6-[[(2S)-2-(ethoxycarbonyl)-4,4-difluoro-1-pyrrolidinyl]methyl]decahydro-, ethyl ester, (3S,4aR,6S,8aR)-, mono(α-hydroxybenzeneacetate) (9CI) (CA INDEX NAME)

CM 1

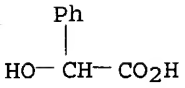
CRN 317844-31-8
CMF C20 H32 F2 N2 O4

Absolute stereochemistry.



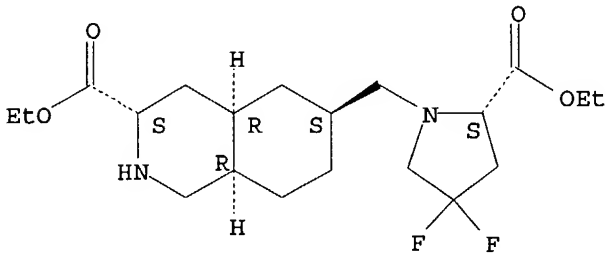

CM 2

CRN 90-64-2
CMF C8 H8 O3



RN 317844-37-4 CAPLUS
CN 3-Isoquinolinecarboxylic acid, 6-[[(2S)-2-(ethoxycarbonyl)-4,4-difluoro-1-pyrrolidinyl]methyl]decahydro-, ethyl ester, dihydrochloride, (3S,4aR,6S,8aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



●2 HCl

=> log y

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| FULL ESTIMATED COST | 16.98 | 172.61 |

| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| CA SUBSCRIBER PRICE | -2.10 | -2.10 |

STN INTERNATIONAL LOGOFF AT 10:55:19 ON 21 SEP 2004